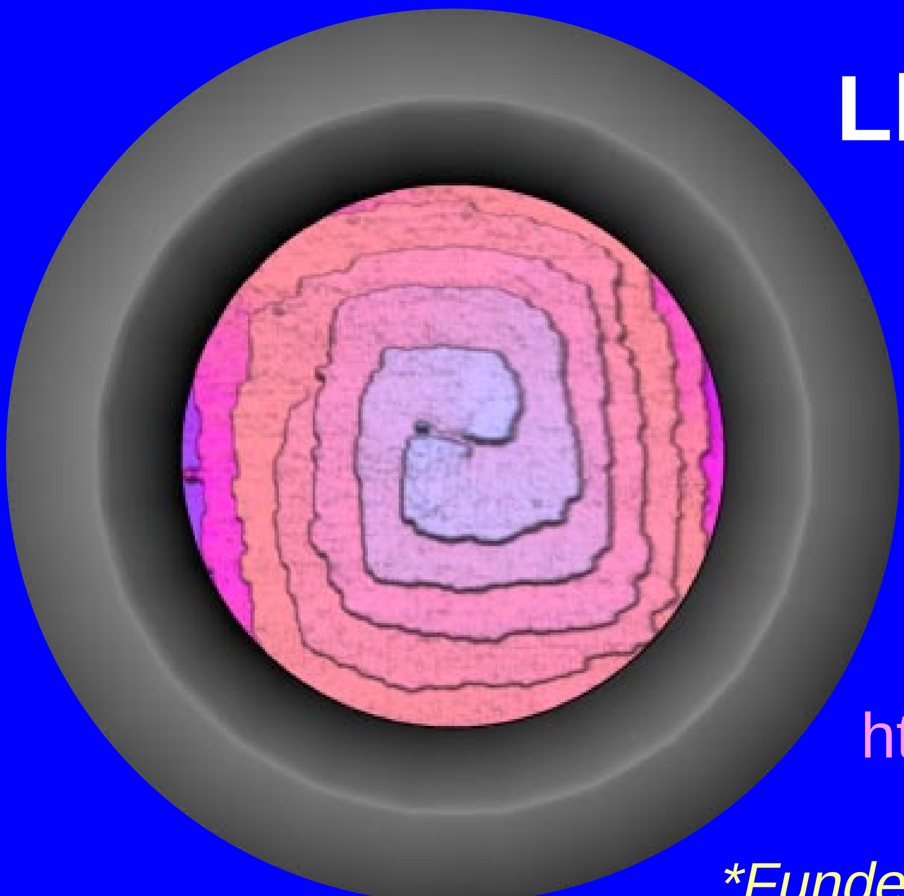
MBE Under the Microscope: An STM View of "6.1 Å" Surfaces and Interfaces*



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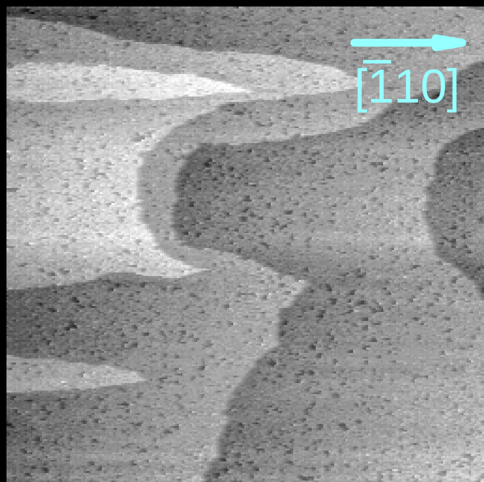
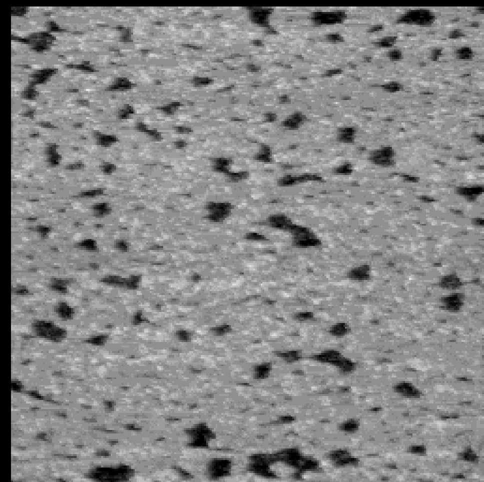
*Funded by ONR, DARPA, and AFRL

Can STM Help MBE?

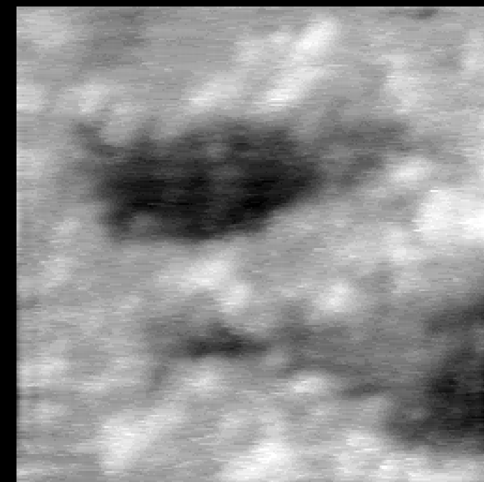
4/10/95: First images – "We'll grow our best GaAs(001)-(2×4)"



1.6 µm × 1.6 µm

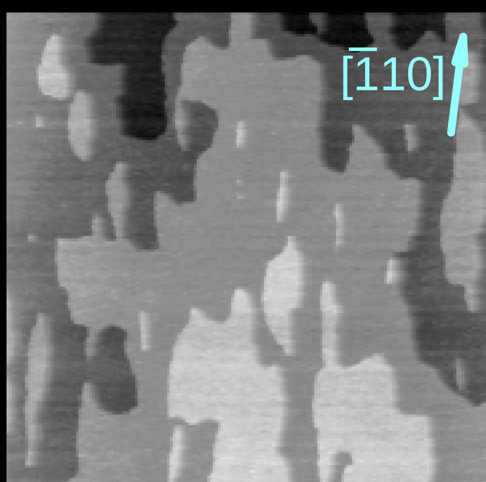


4000 Å × 4000 Å



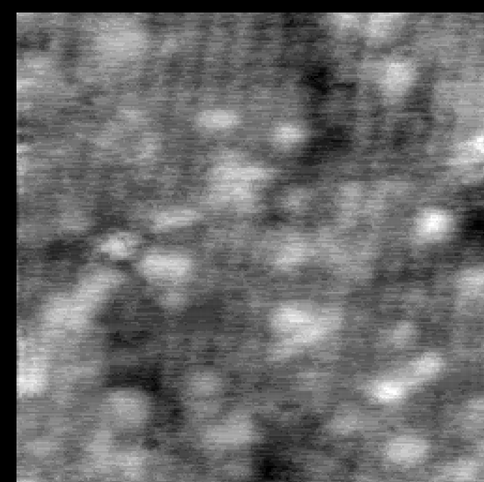
320 Å × 320 Å

NEXT DAY: big pits gone, atomic-scale order visible



1.6 µm × 1.6 µm

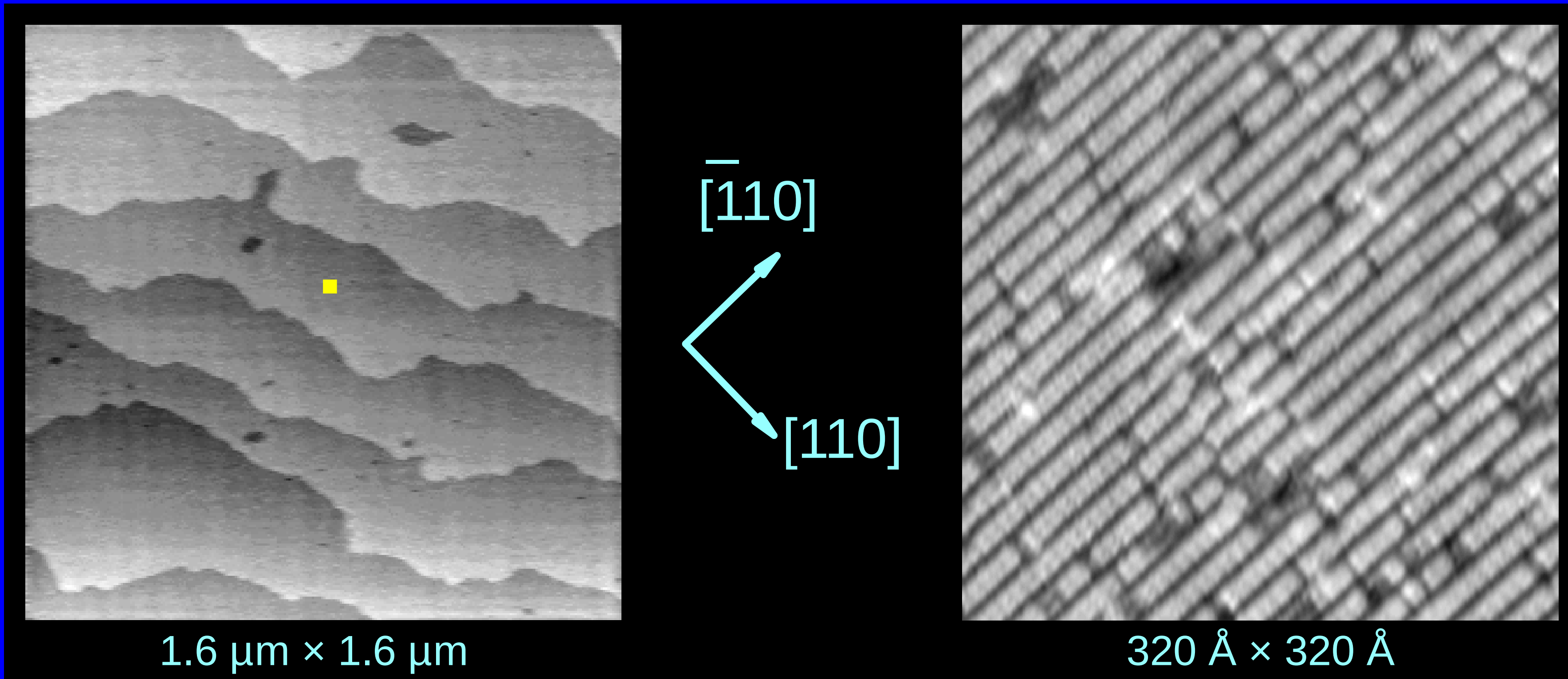
4000 Å × 4000 Å



320 Å × 320 Å

After Two Years of STM/MBE

5/97: Almost ideal terrace morphology, good (2×4)



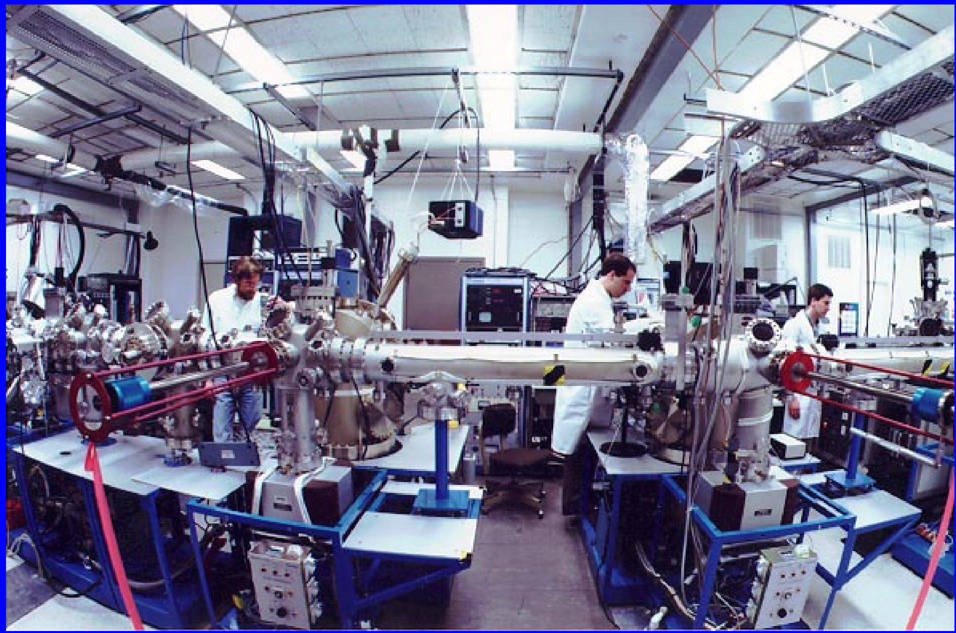
MBE: 1 ML/s at 600 °C, with 30 s interrupts every 90 s.
After ~1 µm, 10 min interrupt to finish.

Cast of Characters

From NRL:

W. Barvosa-Carter
B. R. Bennett
A. S. Bracker
J. C. Culbertson
S. C. Erwin
B. V. Shanabrook
M. E. Twigg
M.-J. Yang

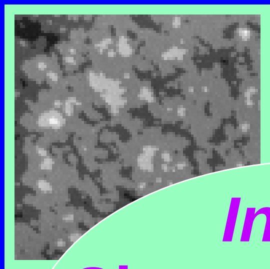
NRL Code 6000 Epicenter

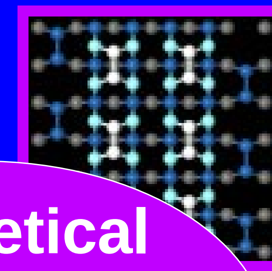


From Elsewhere:

B. Z. Nosho and W. H. Weinberg, UCSB
P. M. Thibado, U. Arkansas
M. B. Weimer, Texas A&M
J. J Zinck, HRL

III-V Device Optimization





In-Situ
Characterization

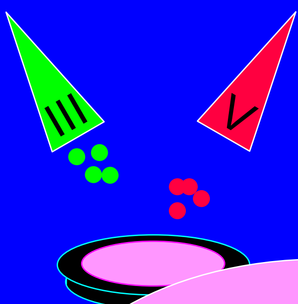
RHEED, XPS, STM

Theoretical
Calculations

LDA, Modeling

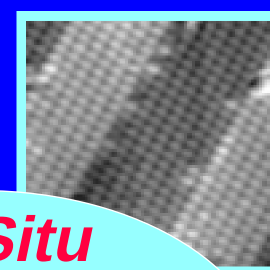
Device
Performance

Electrical
Optical



MBE Growth

Temperature
Flux Rates
Interrupts



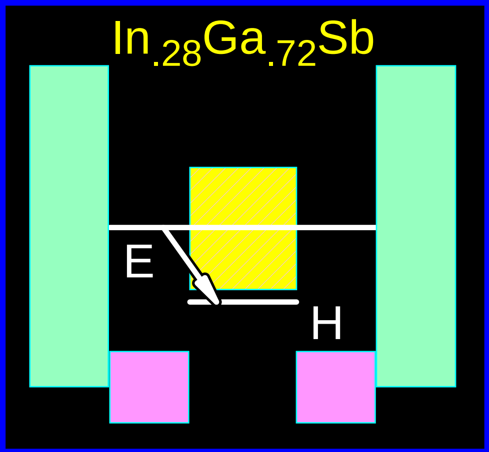
Ex-Situ
Characterization

X-STM X-ray
X-TEM Raman

Requires integrated approach.

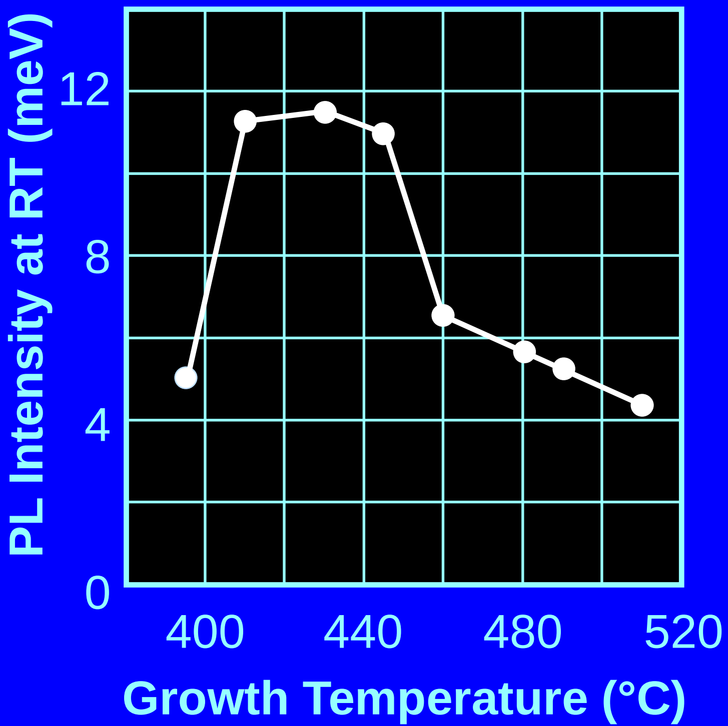
Interface Sensitivity: IR Laser Structures

- AlSb - InAs - InGaSb - InAs Superlattice



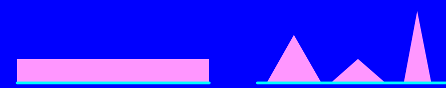
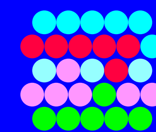
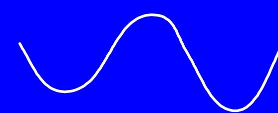
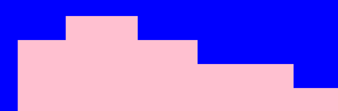
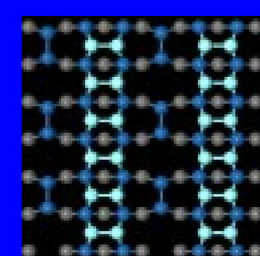
Layer Thickness (ML) vs Wavelength

AlSb	InAs	InGaSb	InAs	λ (µm)
14	8	10	8	**6.8**
14	7	10	7	**5.8**
14	6	10	6	**5.1**
14	5.5	10	5.5	**4.4**



Interfaces Matter!

What Do We Need To Learn?

- Interface roughness – two components
  - Topography: 2D vs 3D growth 
  - Intermixing: during or after interface formation 
- Kinetics vs. Thermodynamics 
  - Interplay between energy *barriers* and energy *differences*
- Continuium vs. Atomistic 
  - Island/Step edge dynamics
  - Surface reconstruction: anisotropy, III/V stoichiometry 

Control via growth methods, e.g. MEE, interrupts.

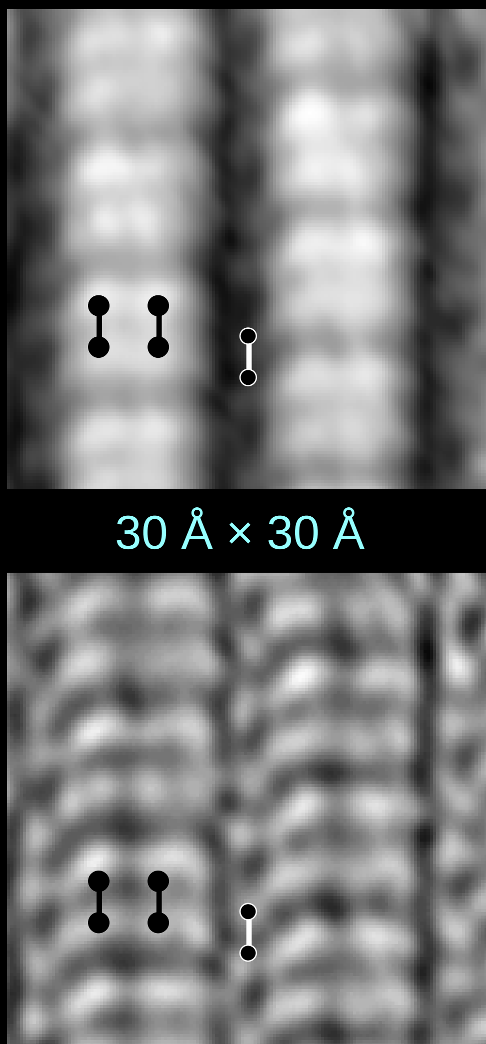
Start At The Atom: Surface Reconstructions

- Focus on device-growth conditions: ***V-rich***
- InAs(001)-(2×4), c(4×4): like GaAs
  - Nominally obeys ***Electron Counting Model*** (ECM): *In-dangling bonds (db's) empty, As-db's filled*
- AlSb vs. GaSb(001): role of material properties vs. lattice constant (AlSb 0.7% larger)
  - AlSb: only (1×3), c(2×6) RHEED reports
  - GaSb: (1×3), c(2×6), (1×5), (2×5) by RHEED, previous STM of c(2×6)

InAs(001)-(2×4) Reconstruction

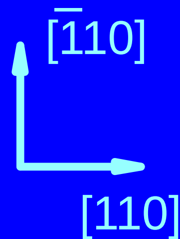
GaAs(001)-"(2×4)"

Filled State Image



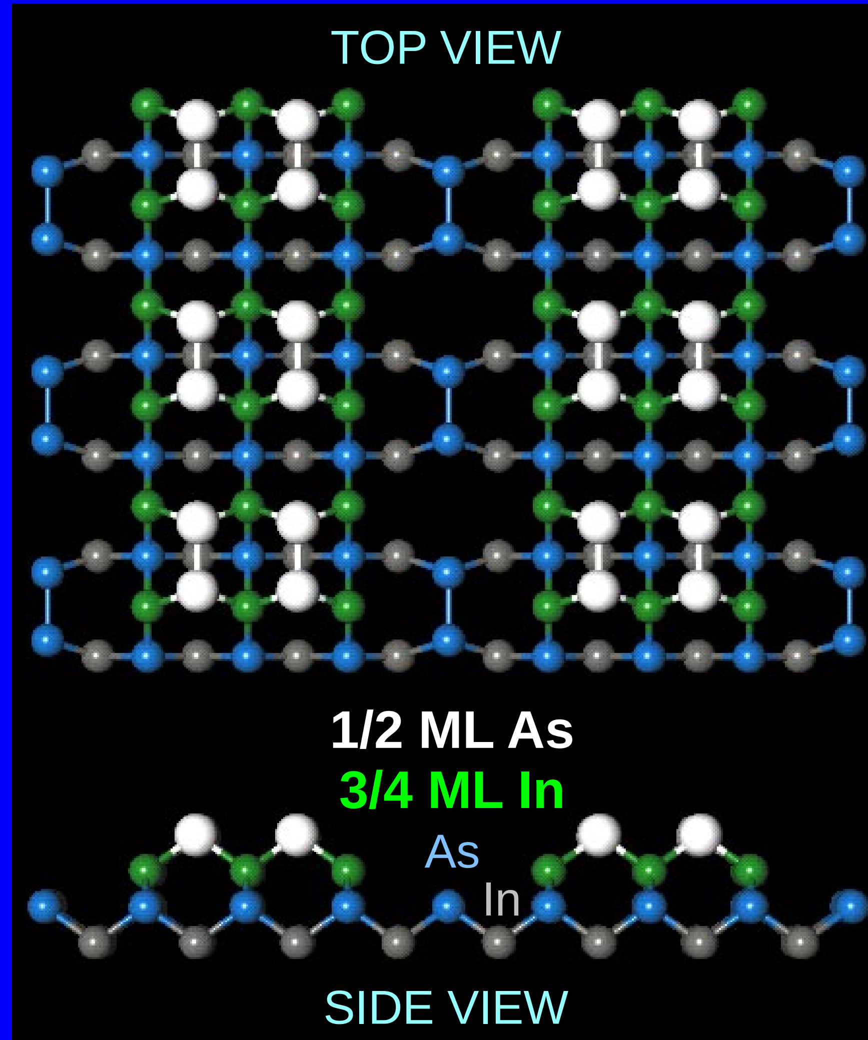
30 Å × 30 Å

High-Pass Filtered



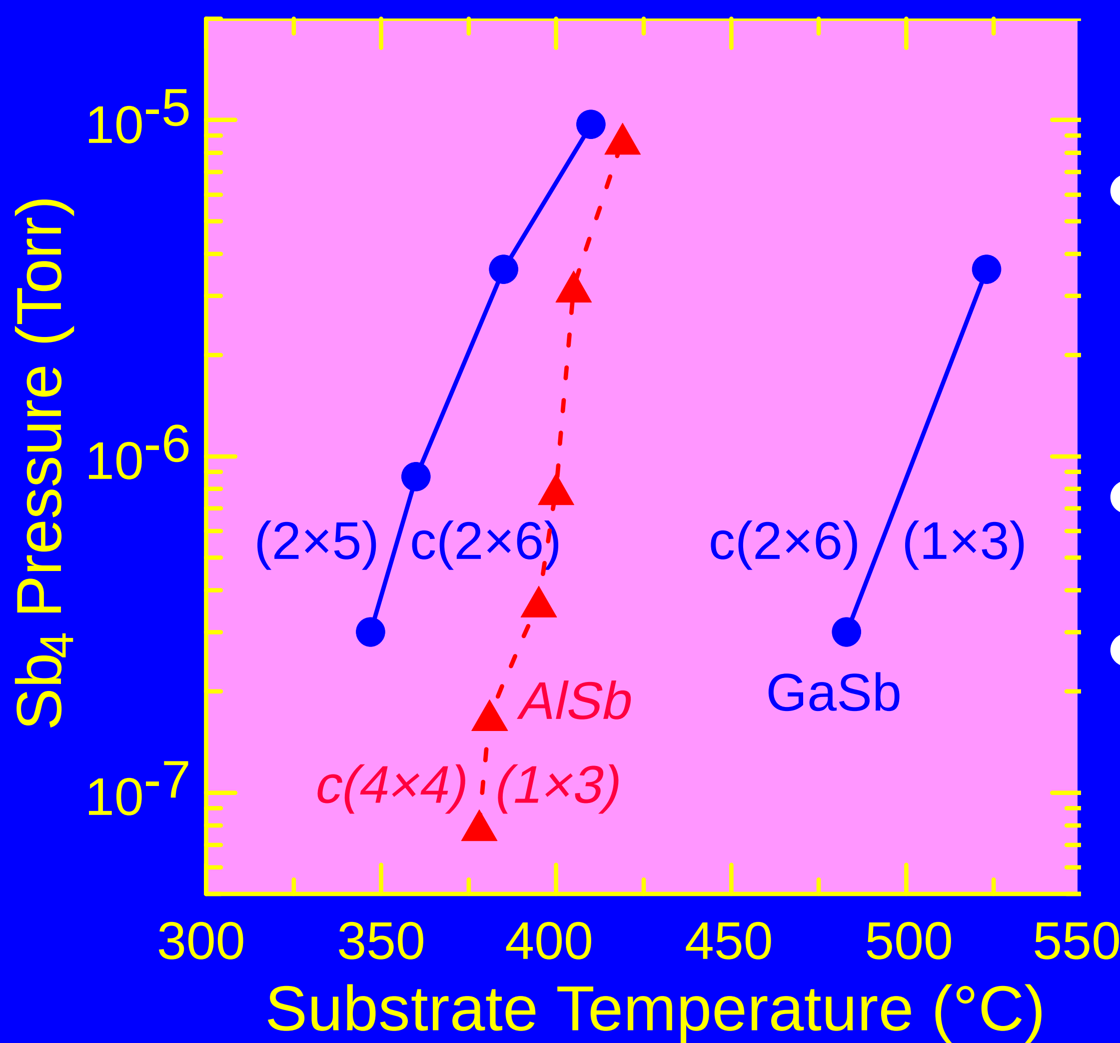
0.5 ML As
on
0.75 ML In

III-V(001)-β2(2×4)



Follows electon counting model.

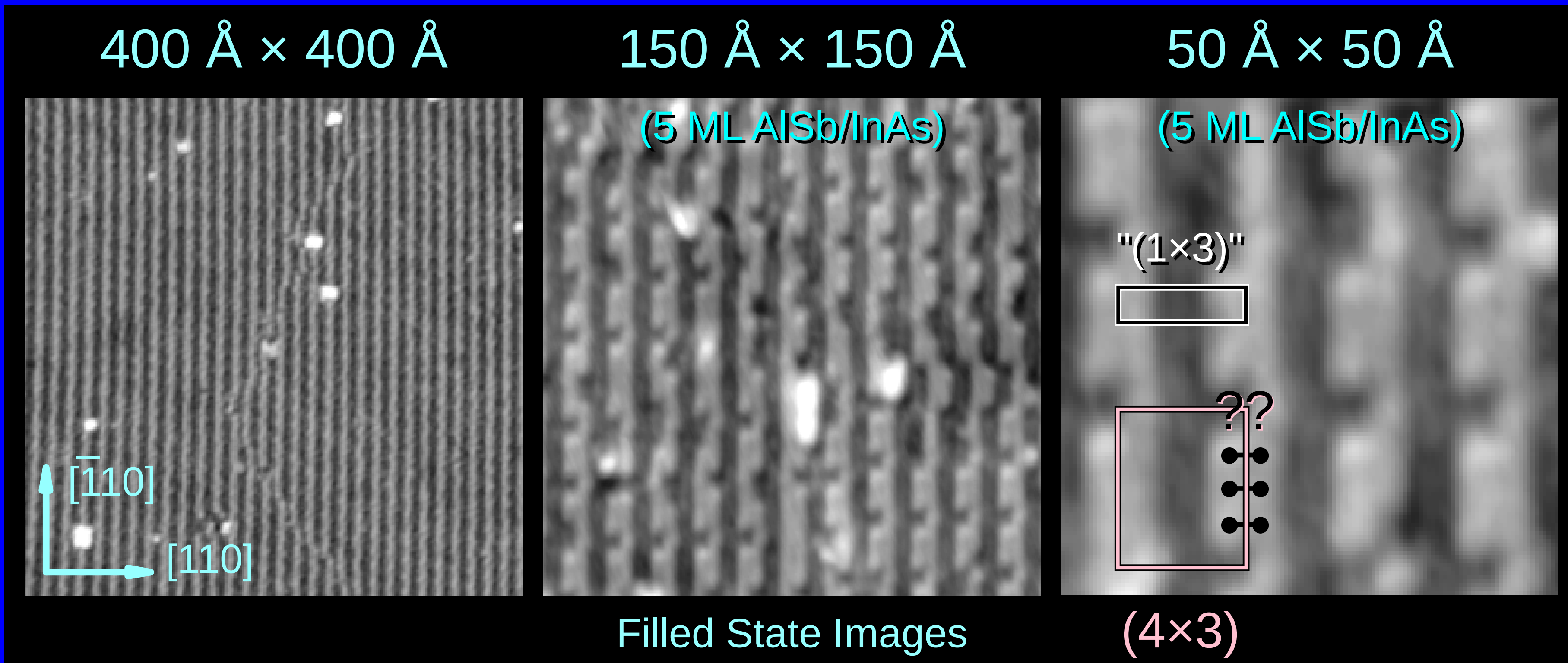
GaSb-AlSb RHEED Structure Diagram



- GaSb: (1×3) - c(2×6) - (2×5): under optimal conditions no (1×5)
- AlSb: (1×3) - c(4×4)
- AlSb(001)-c(4×4) for first time

What are structures, what makes them different?

AlSb(001)-"(1×3)" Reconstruction

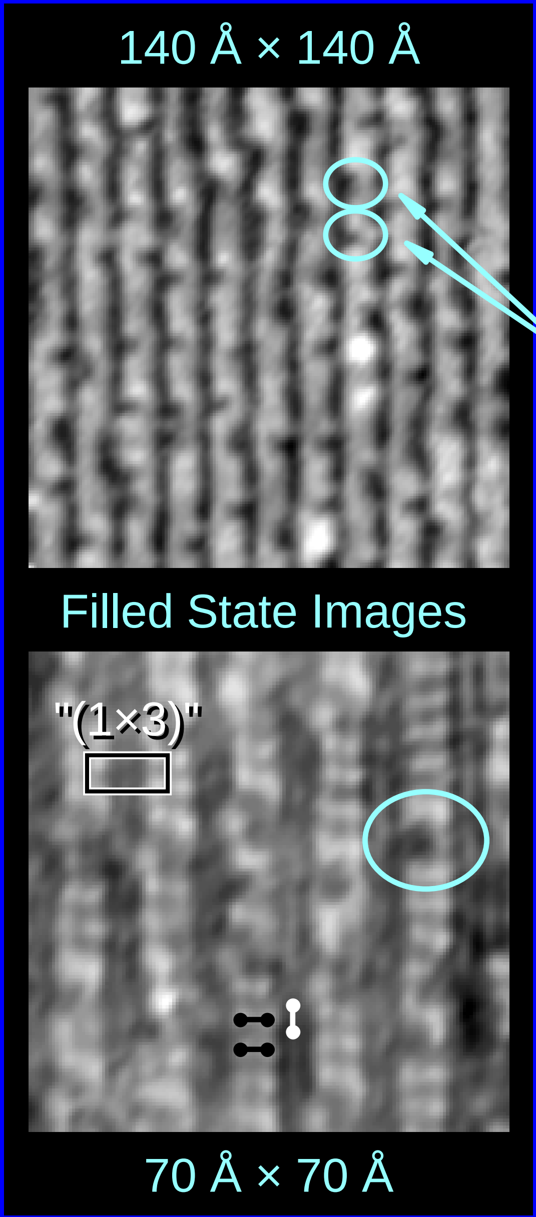


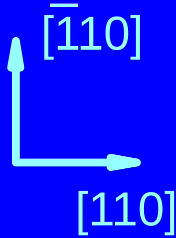
- MBE: grown at 500 °C on GaSb, >10 min interrupt at end
- Only (1×3) seen in RHEED

Quasi-periodic defects make local (4×3) domains.

III-Sb(001)-"(1×3)" Reconstruction

GaSb(001)-c(2×6)

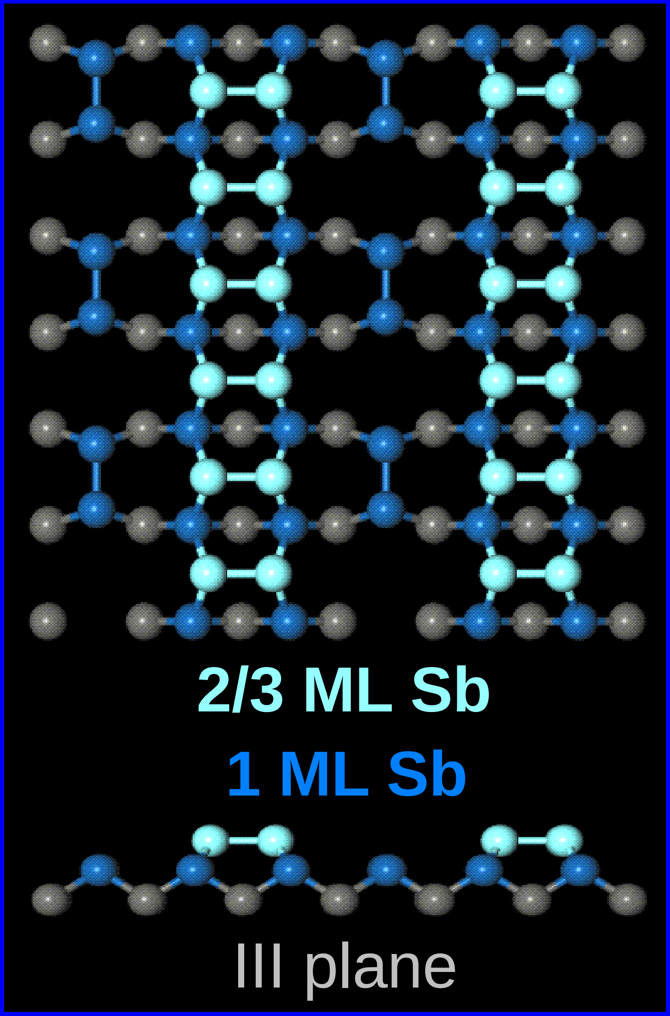




Quasi-periodic defects

1.66 ML Surface Sb

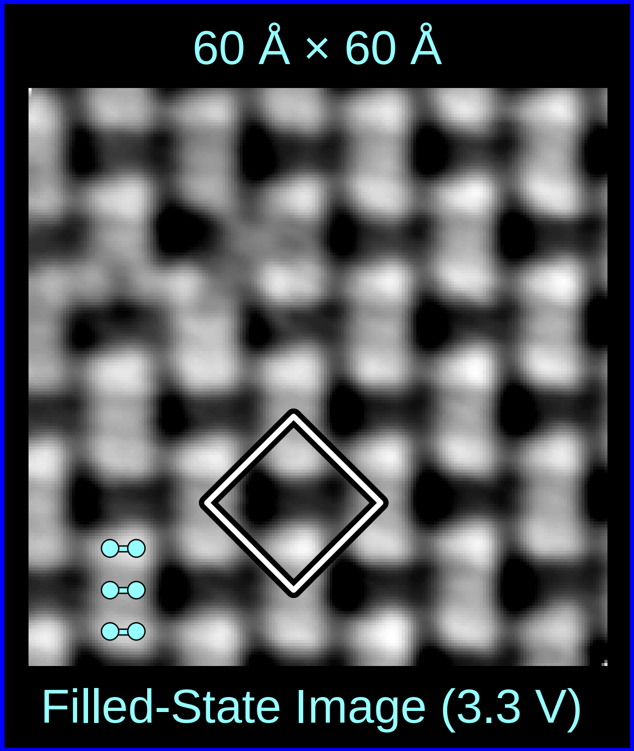
III-Sb(001)-c(2×6)

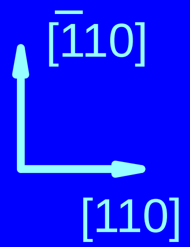


(Al,Ga,In)Sb "(1×3)" all look similar.

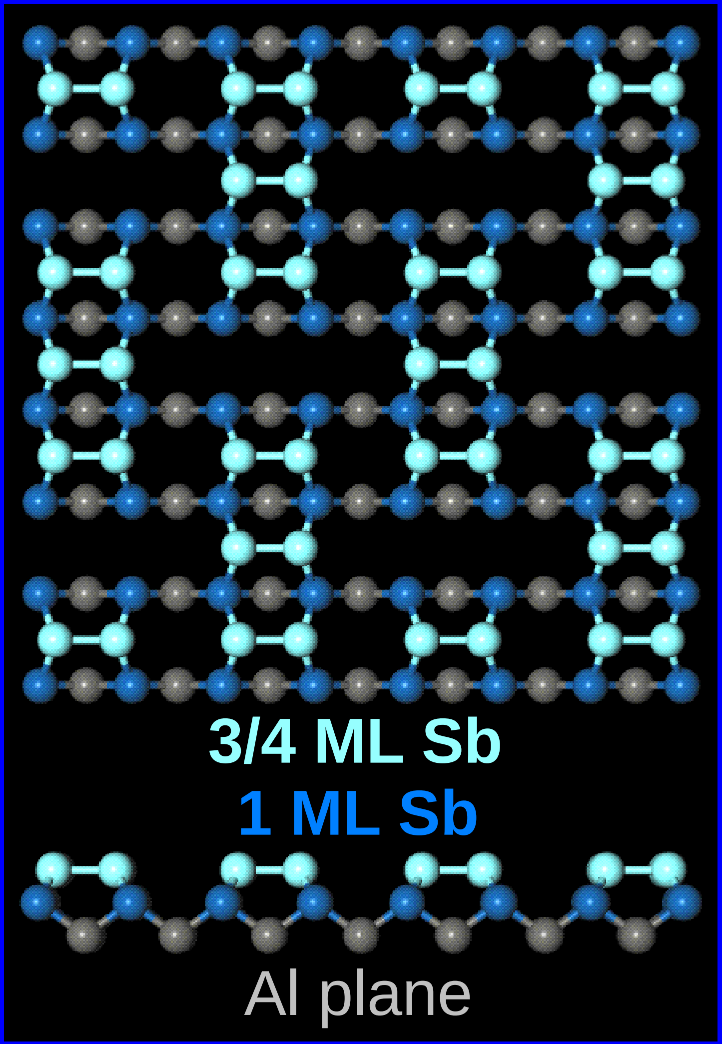
Actual structure more complex?

AlSb(001)-c(4×4) Reconstruction





1.75 ML Surface Sb

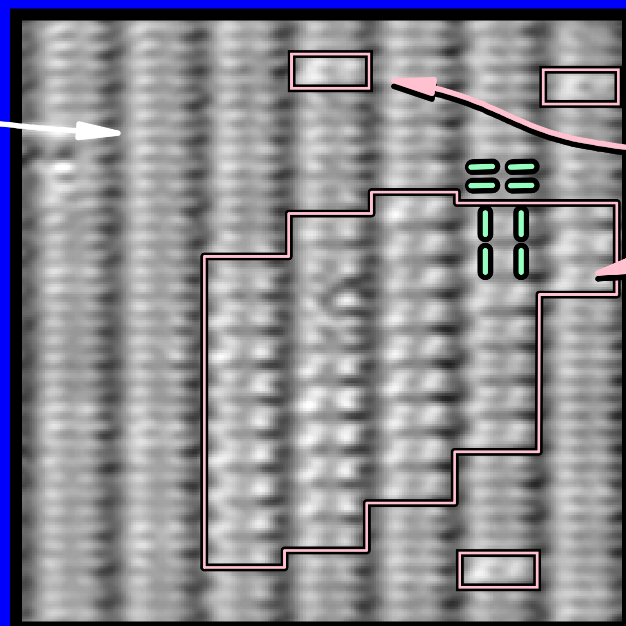


Simple dimer row structure: like ***all other*** III-V's (except GaSb).

Follows ECM: expect insulating surface.

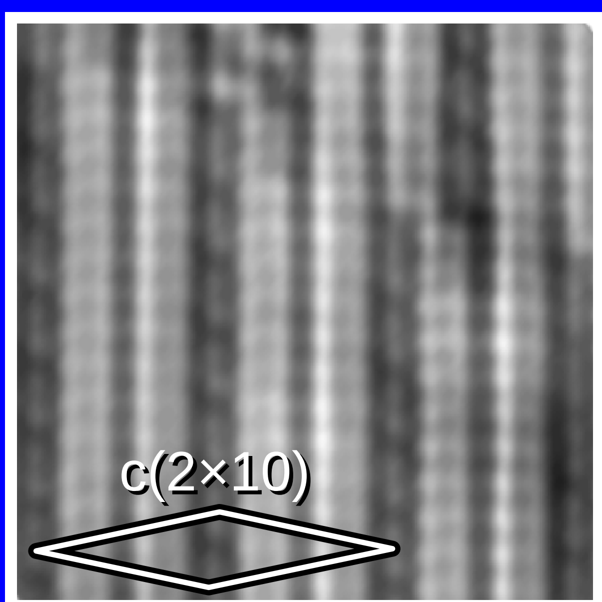
GaSb(001)-"(2×5)" Reconstructions: STM

Two (n×5)-like structures
(atypical mixed-phase shown)



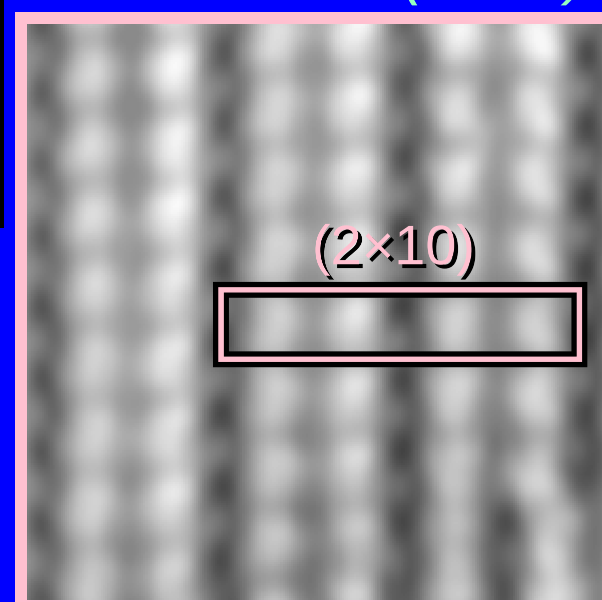
150 Å: Filled States (2.4 V)

On high-T side of
"×5" range, c(2×10)



65 Å: Filled States (1.8 V)

At lower T's,
different (2×10):
features rotate,
are ~1 Å higher
than on c(2×10)



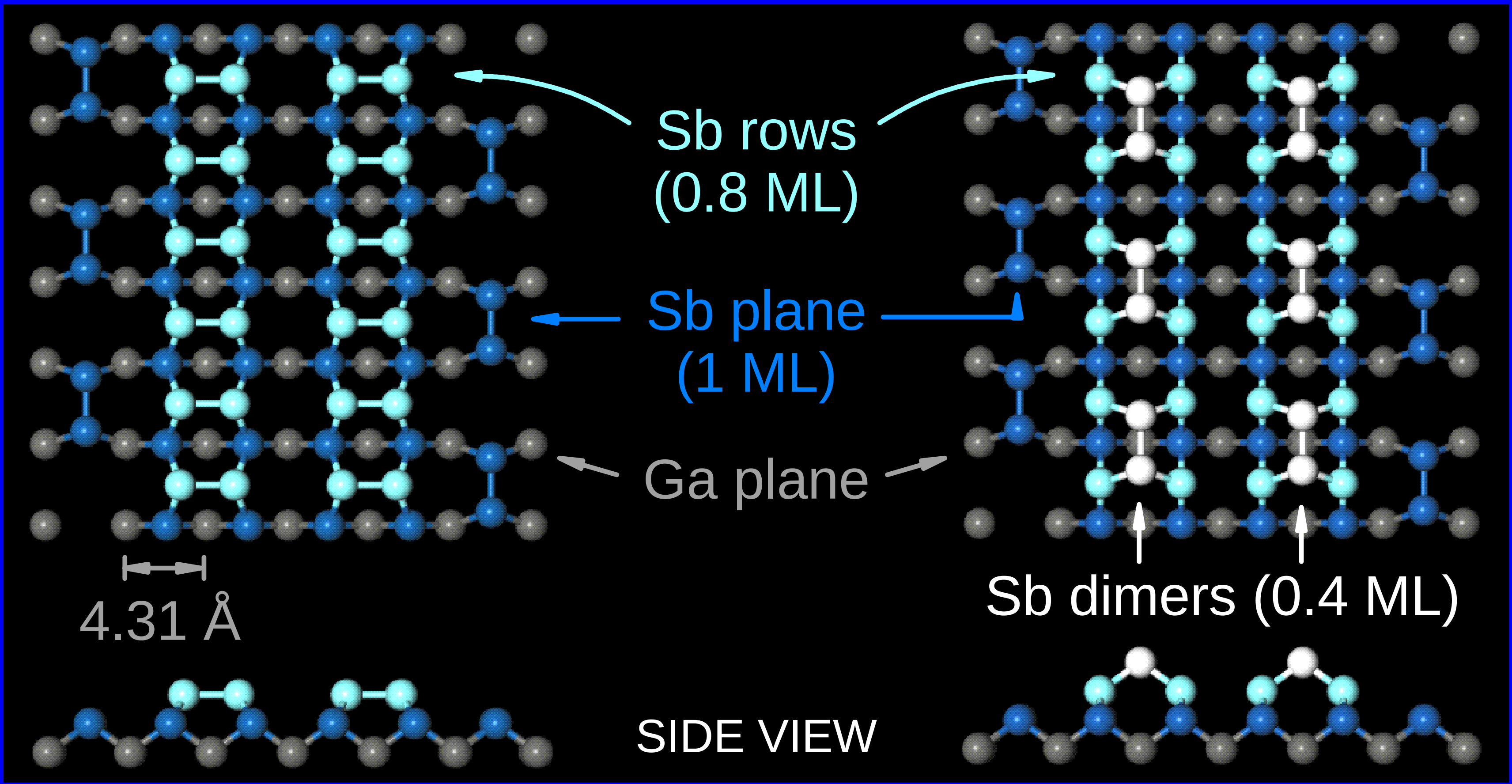
65 Å: Filled States (0.4 V)

[$\bar{1}$10]

[110]

GaSb(001)-"(2×5)" Models

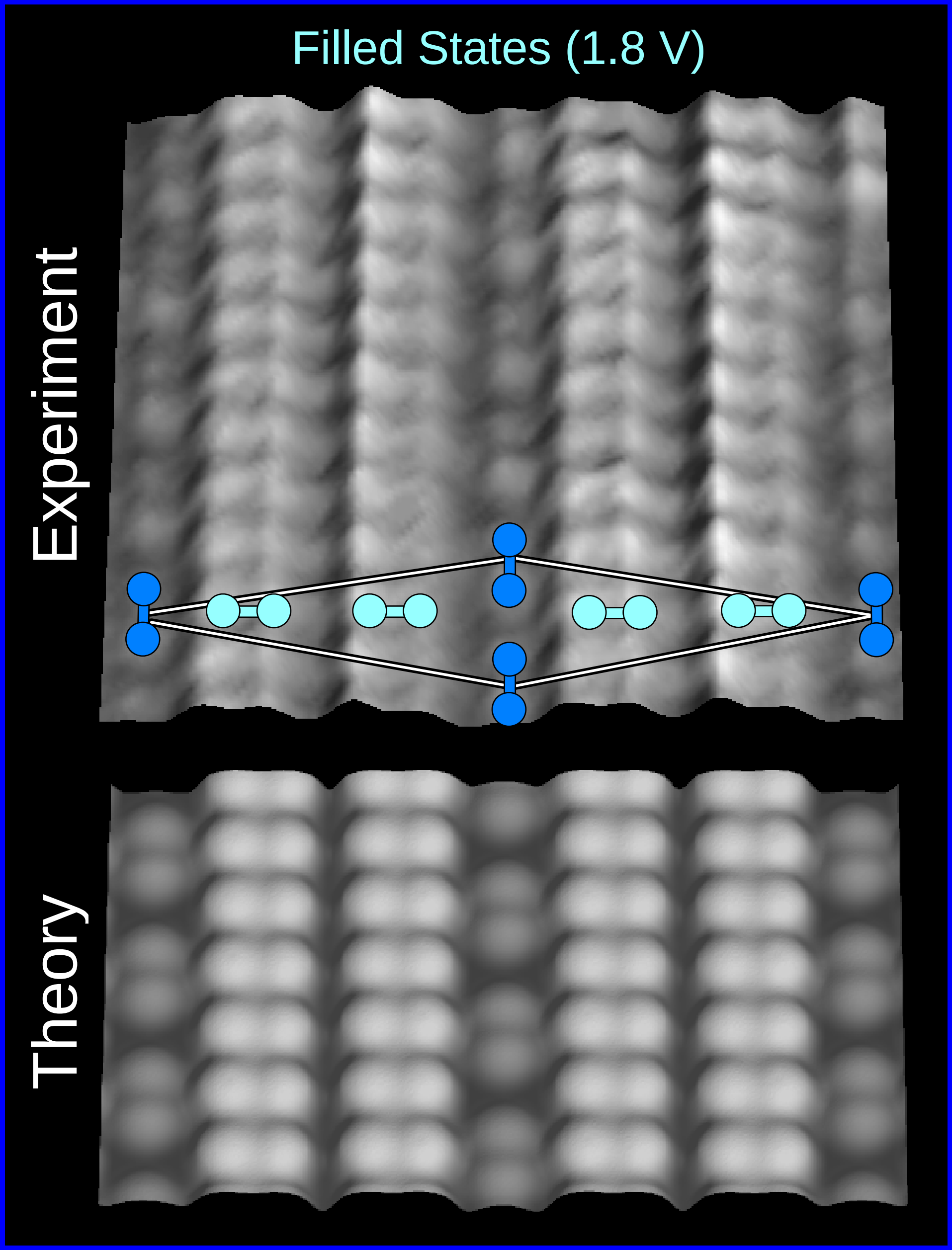
c(2×10): **1.8 ML Sb** (2×10): **2.2 ML Sb**



Three extra *e*'s/(2×5): **expect metallic surfaces.**

Both models violate electron counting model!

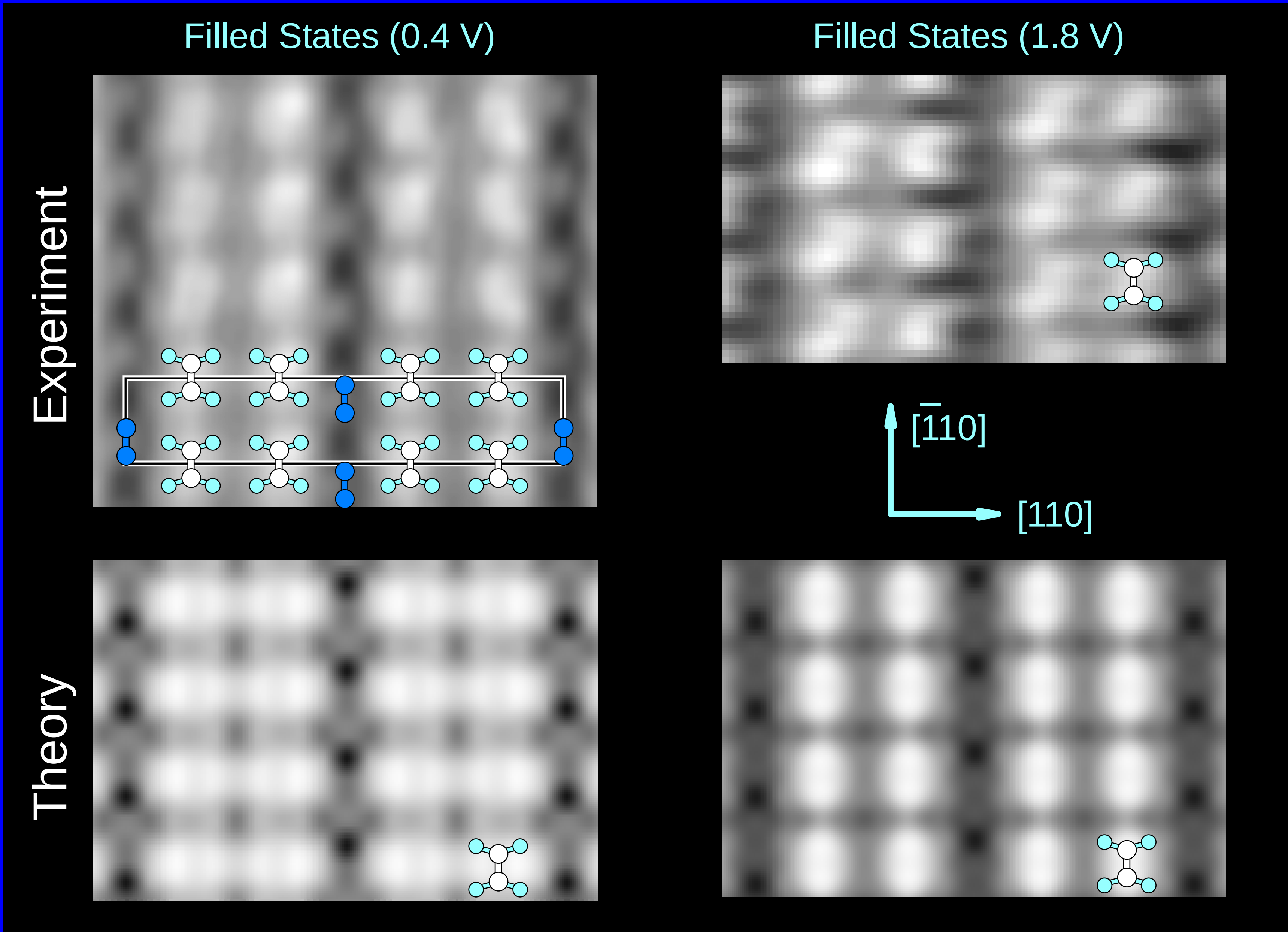
GaSb(001)-c(2×10): Experiment vs. Theory



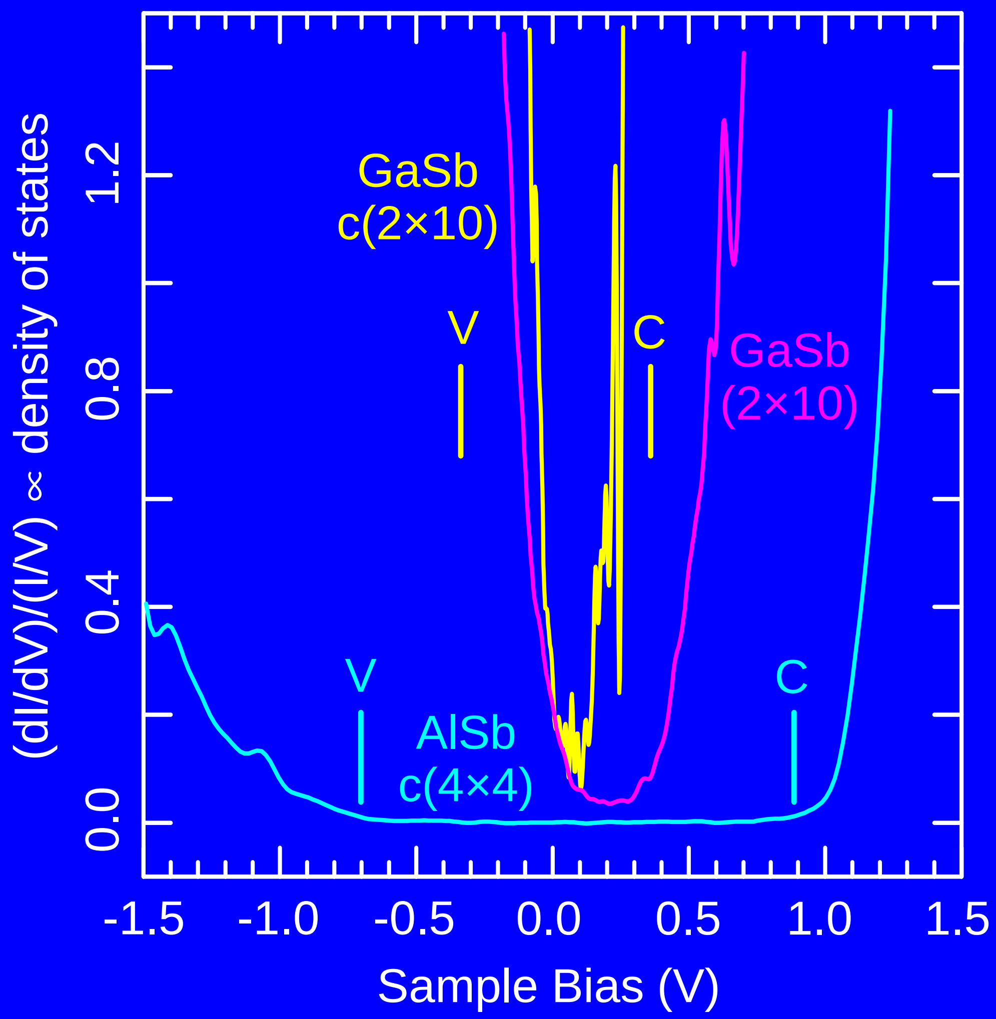
- First-principles, electronic-structure calculation (LDA)
- Local-state density $\rho(r,\varepsilon)$ computed from wave functions
- At each r, integrate $\rho(r,\varepsilon)$ over filled or empty states
- Simulate constant current STM image by surface of constant integrated $\rho(r,\varepsilon)$

Similar results for (2×10).

GaSb(001)-(2×10): Experiment vs. Theory



AlSb and GaSb(001) Tunneling Spectroscopy



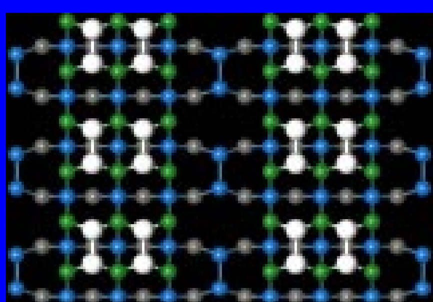
- AlSb insulating, as expected from ECM
- GaSb ***weakly metallic: non-zero conductivity at all bias voltages***
- Theory shows occupied conduction band states on GaSb

Electron counting model violated on GaSb(001).

"6.1 Å" V-Terminated Reconstructions

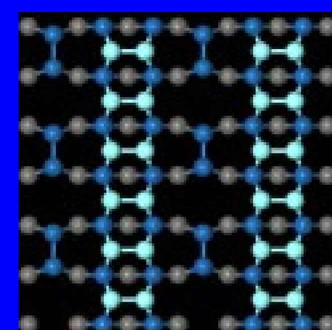
InAs		GaSb		AlSb
c(4×4)	1.75 As/1.0 In	(2×10)	2.20 Sb/1.0 Ga	c(4×4)
(2×4)	0.5 As/0.75 In	c(2×10)	1.80 Sb/1.0 Ga	"c(2×6)"
		c(2×6)	1.66 Sb/1.0 Ga	

- GaSb (2×10)'s violate ECM – weakly metallic



(2×4)

InAs ← *Growth Surfaces* → GaSb / AlSb

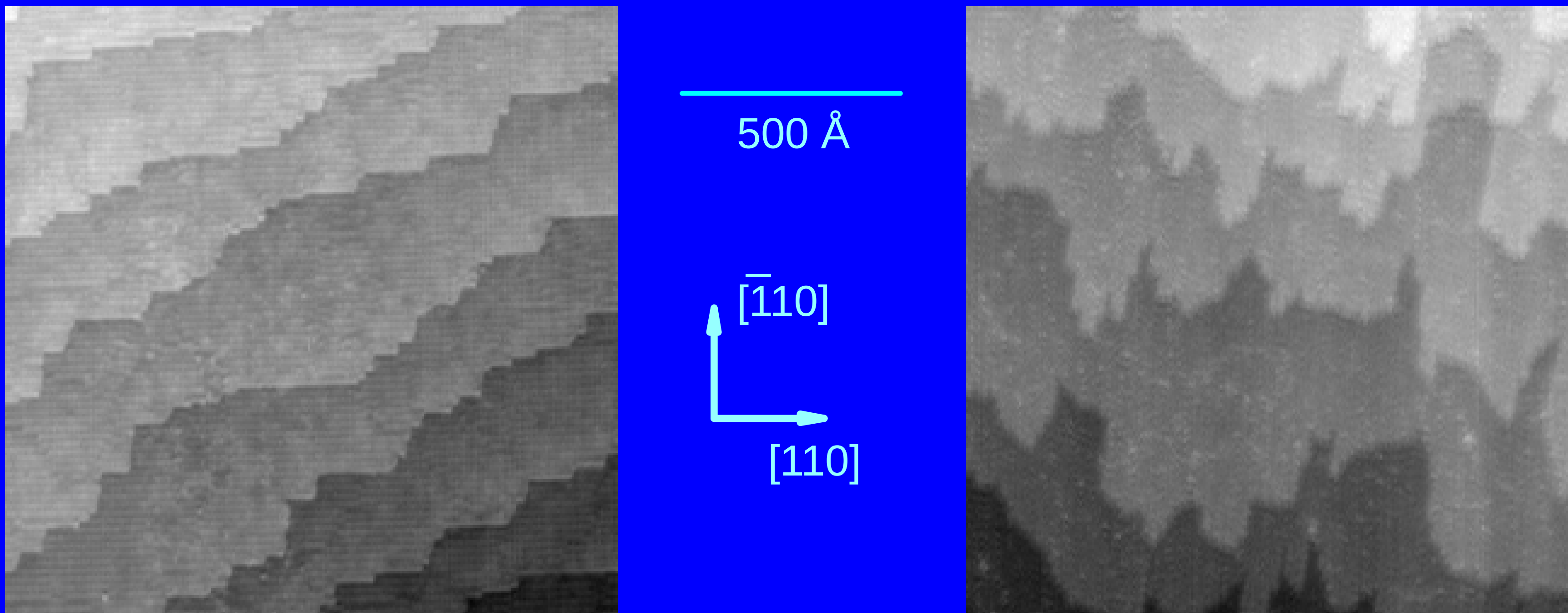


c(2×6)

Do reconstructions impact devices?

Impact of Reconstruction on Step Structure

GaSb(001)-c(2×10) InAs(001)-(2×4)



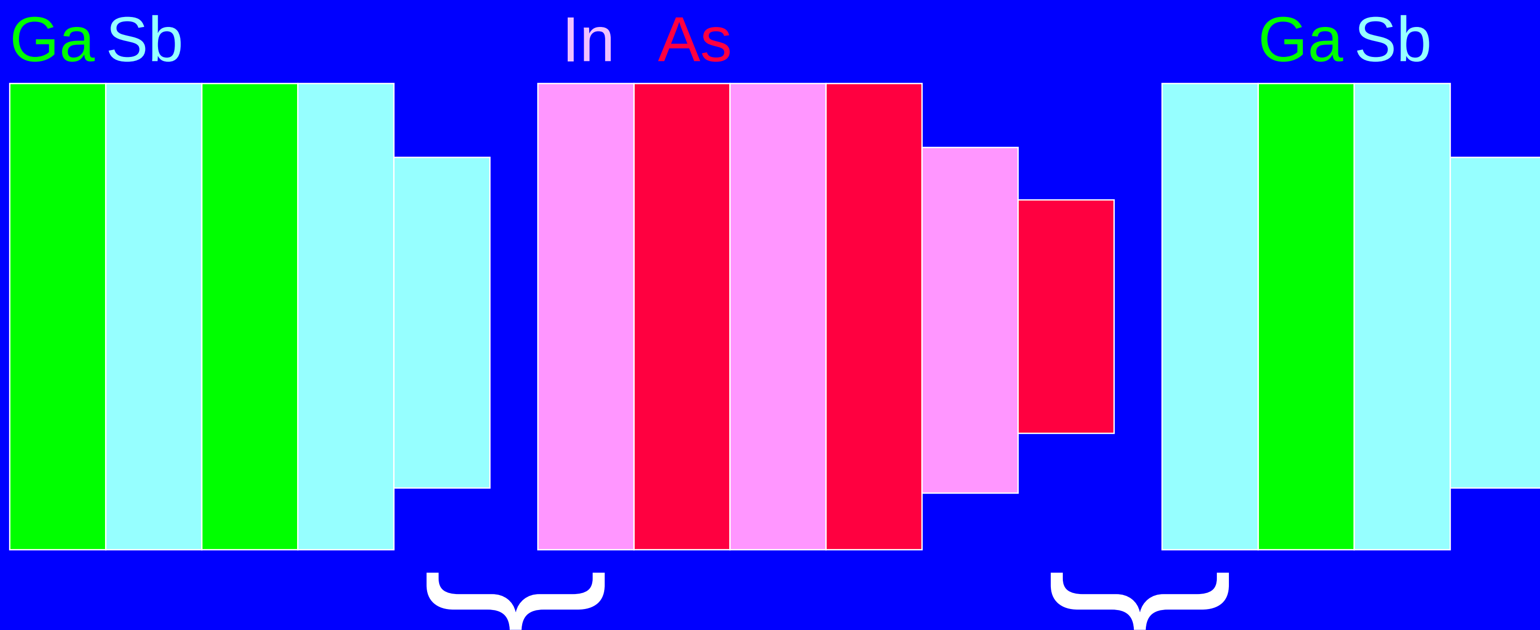
Continous double dimer rows
=> high kink energy
=> straight steps along $[\bar{1}10]$

Different dimer row structure
=> lower kink energy
=> rougher step edges

Implications for: tilted SL, quantum wire growth; electronic mobility anisitropy

Impact of Reconstruction on III-V Heterostructure Interfaces: GaSb/InAs

MBE Growth Direction →

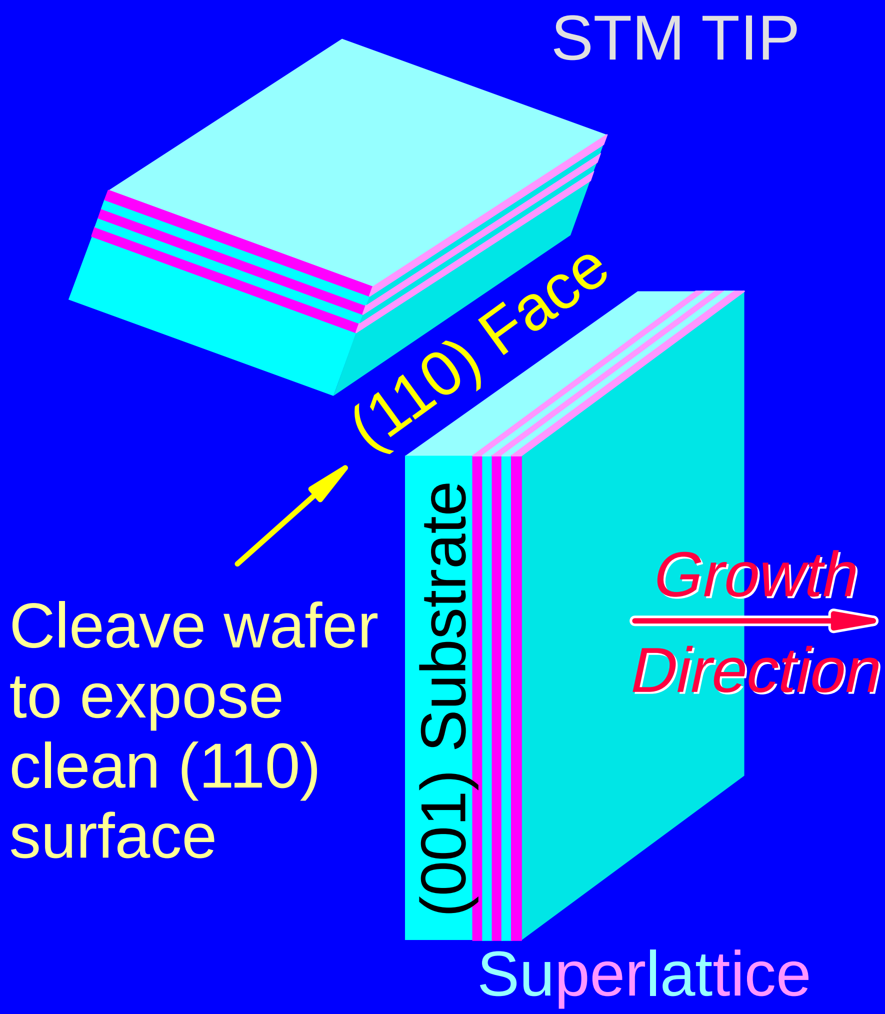


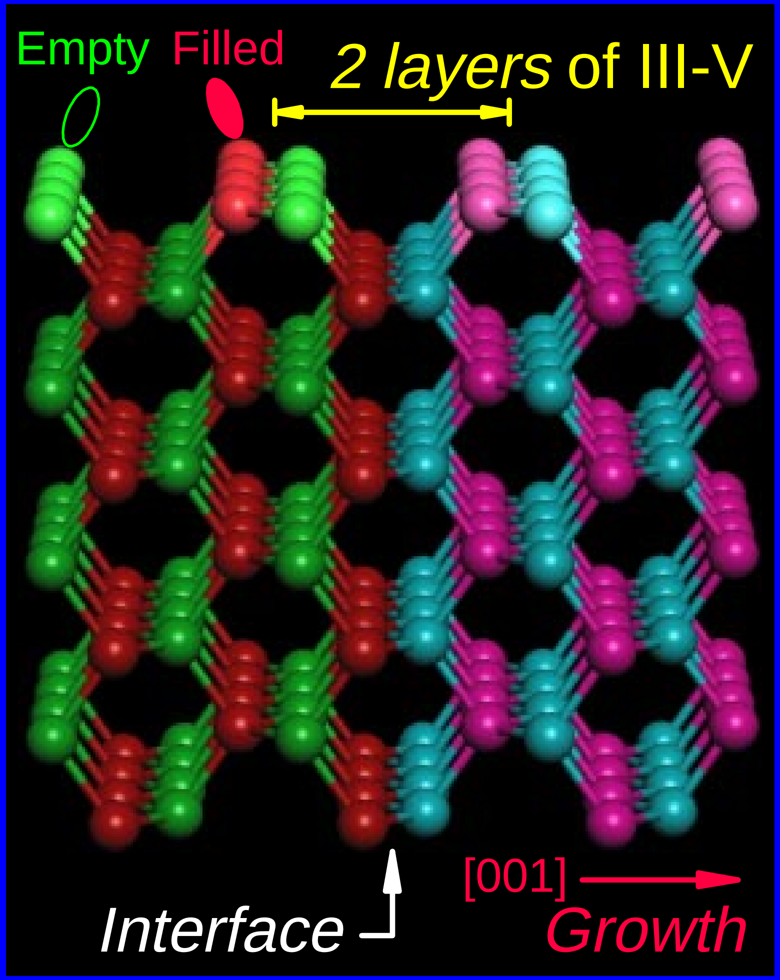
GaSb(001)-c(2×6)
Sb rich (1.66 layers) =>
intermixing at interface?

InAs(001)-(2×4)
As deficient (0.5 layers) =>
intermixing at interface?

Use MEE for InSb interface bonds.

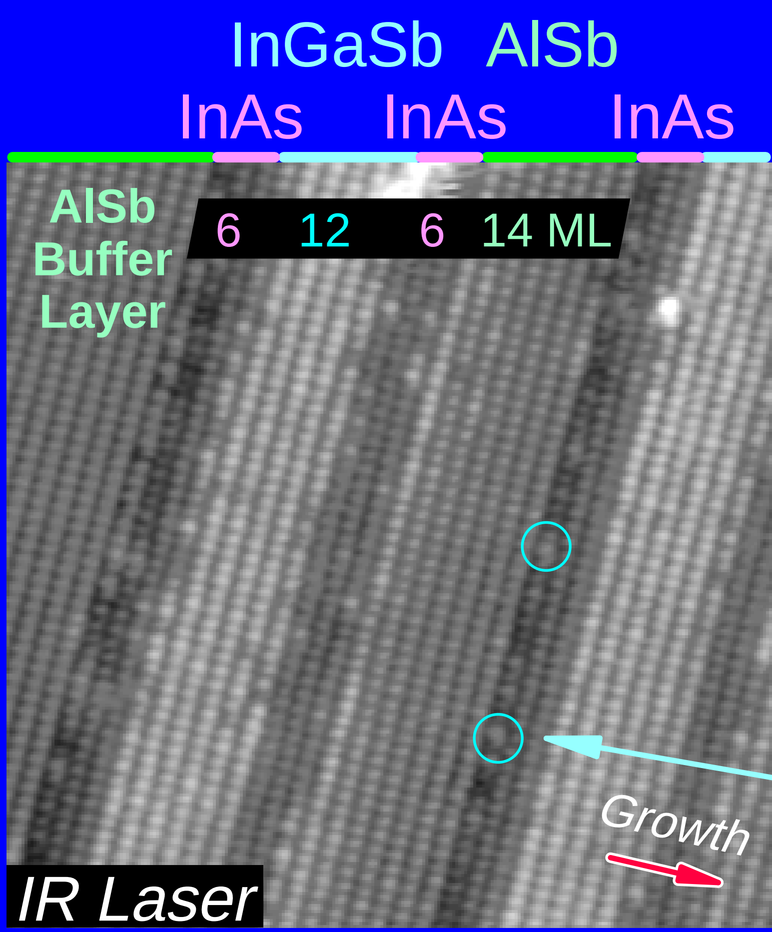
Cross-Sectional STM of (110) Surfaces



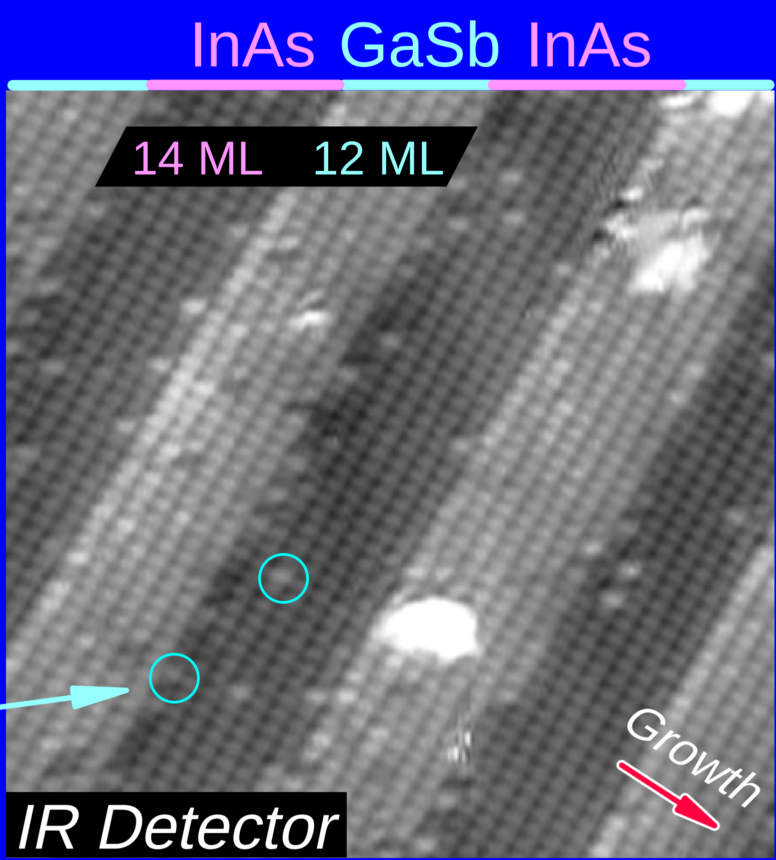


Only see every-other III (empty) or V (filled) layer.

X-STM of "6.1 Å" Superlattices



Filled States: As/Sb sublattices



Sb in InAs

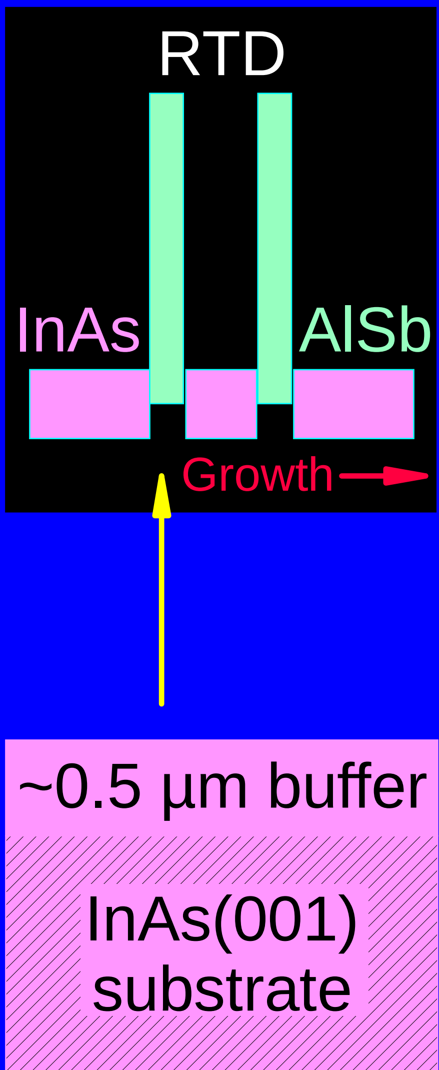
AlSb/InAs ≤2 ML

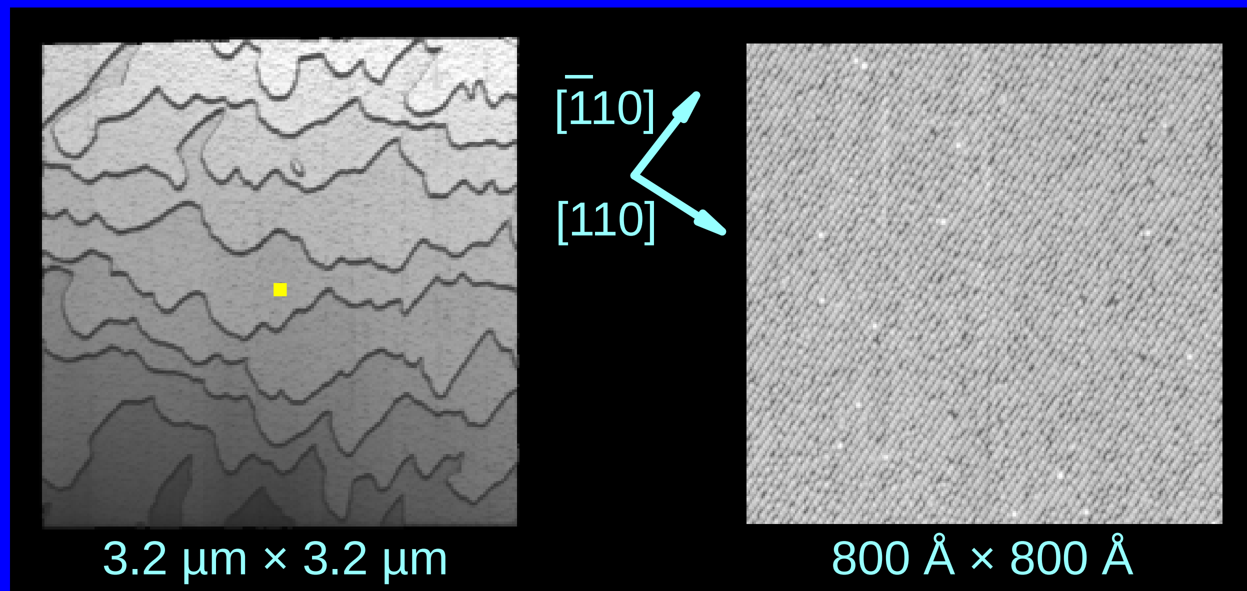
GaSb/InAs ≤2 ML

Intermixing at IIISb/InAs, "abrupt" at InAs/IIISb.

Evolution of InAs/AlSb/InAs RTD Interfaces

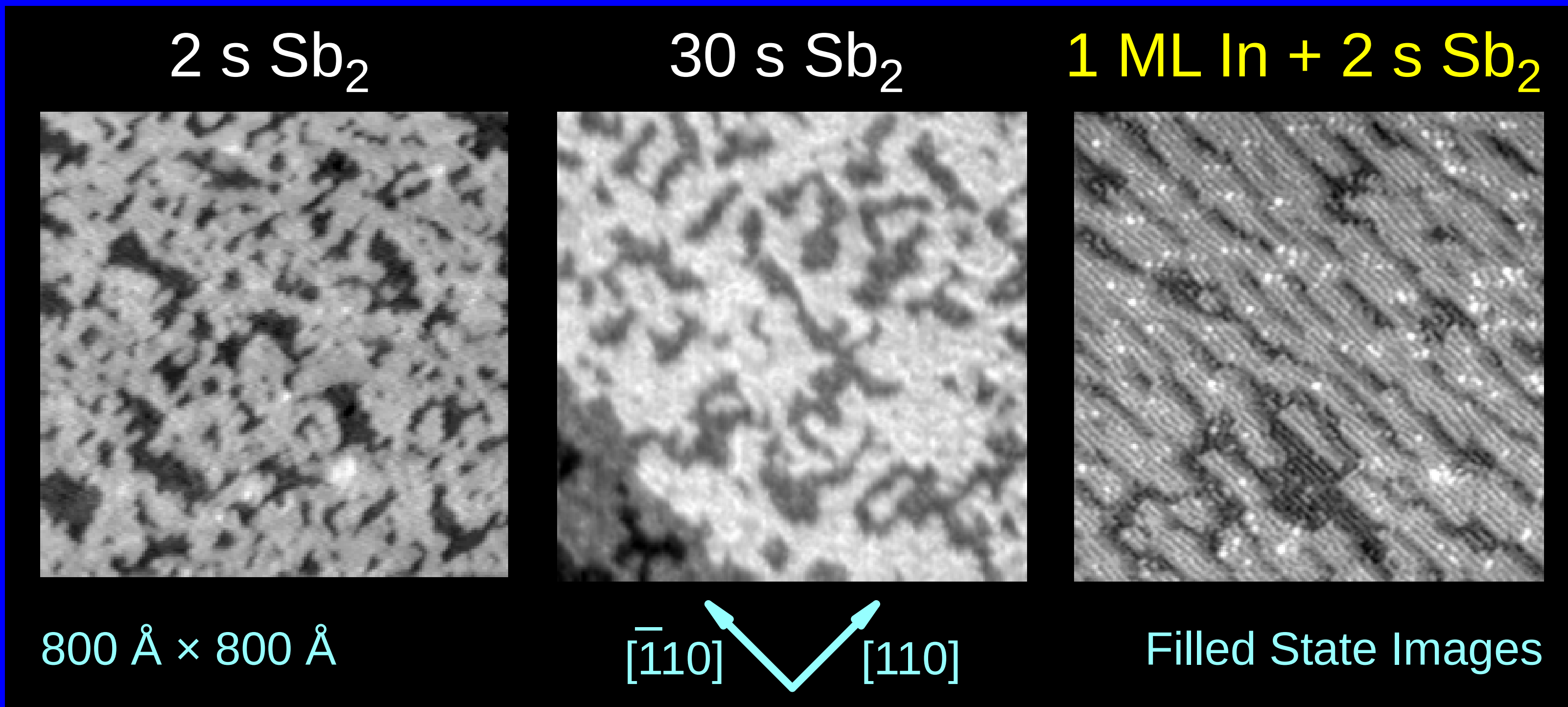
InAs(001)-(2×4) Buffer Layer



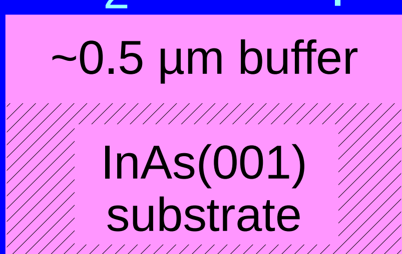


- Nearly ideal surface
- ~1 µm-wide terraces => 0.05° miscut
- MBE: 1 ML/s at 500 °C, 30 s interrupts every 90s, 10 min interrupt after ~1 µm

Sb_2 on InAs(001)-(2×4) at ~400 °C



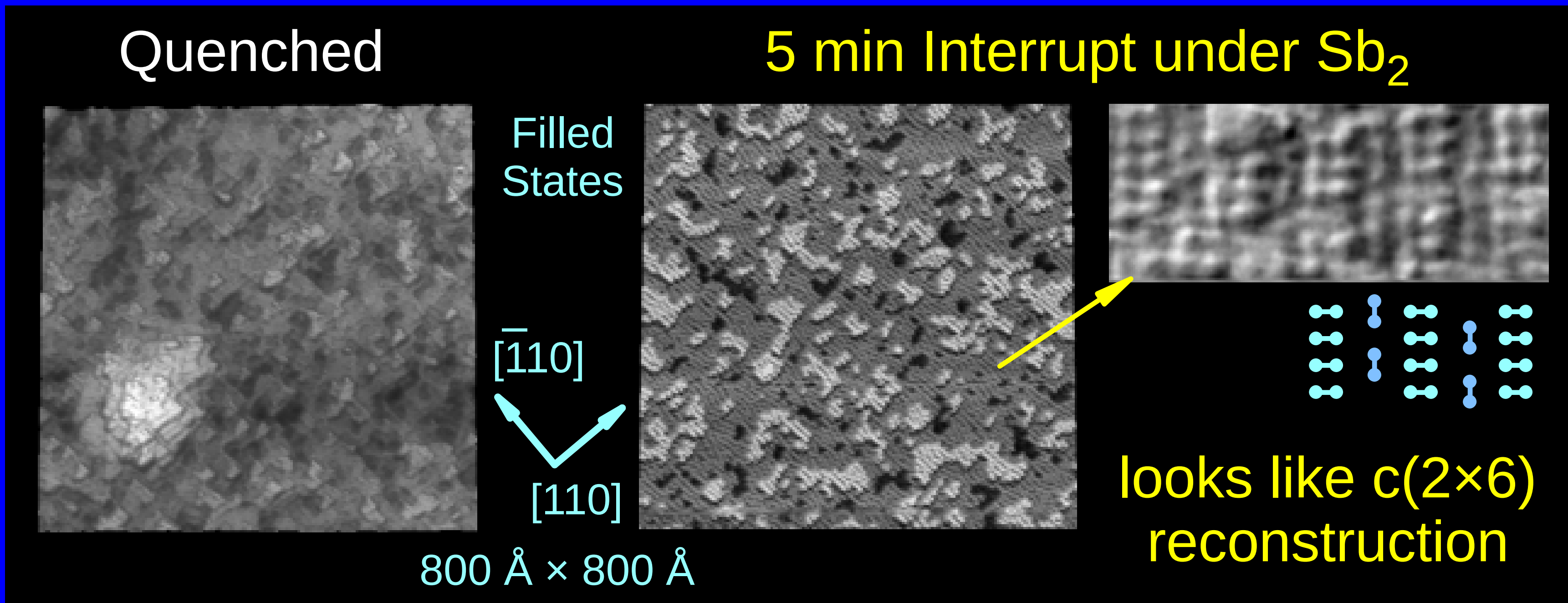
Sb_2 Interrupt



- Want InSb-like bonds at interface
- Surface has InSb "(1×3)"-like reconstruction

Sb very reactive: creates 2-level surface with 25% vacancy islands.

5 ML AlSb on InAs at ~400 °C



5 ML AlSb

1 ML In + Sb_2

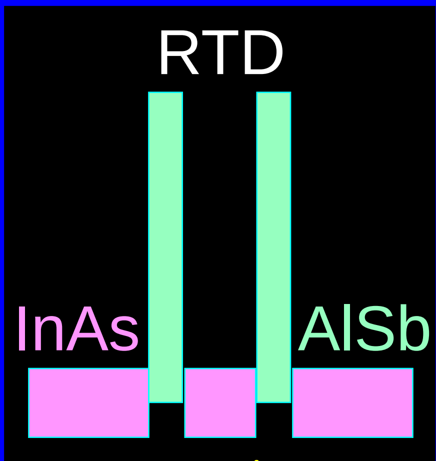
~0.5 µm buffer

InAs(001) substrate

- Addition of AlSb epilayer roughens surface to 3 levels

Interrupt required for well-defined islands and atomic-scale order.

22 ML InAs on AlSb/InAs at ~400 °C



30 s Sb_2

22 ML InAs

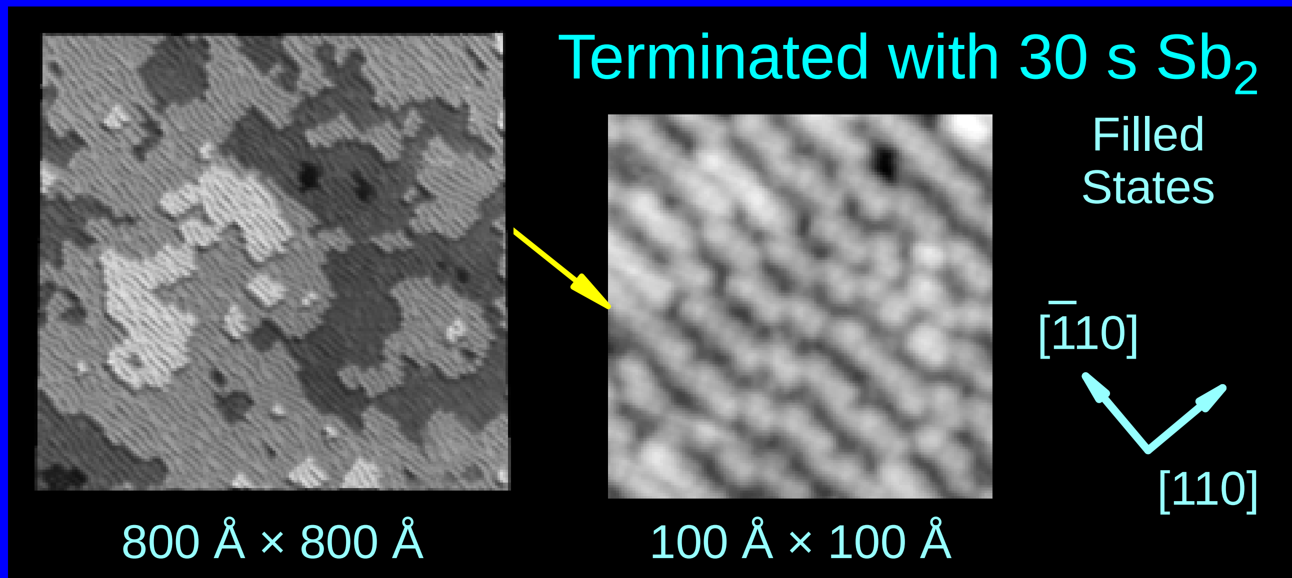
5 min interrupt

5 ML AlSb

1 ML In + Sb_2

~0.5 µm buffer

InAs substrate

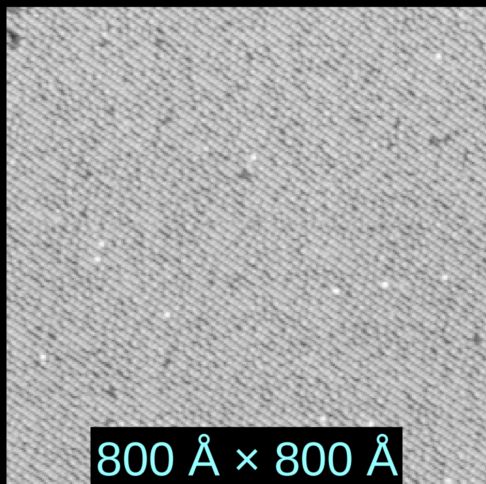


- Represents interface after first barrier
- Now 5 surface levels (but mostly 3)
- Disordered "(1×3)" on surface

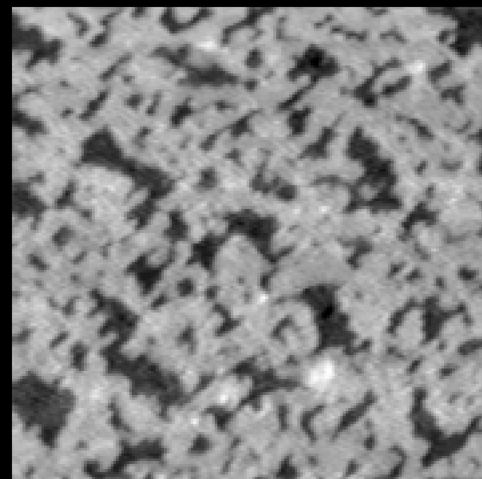
Much different than starting Sb/InAs; history + lower temperature.

Origins of Interface Roughness: Sb/InAs

InAs(001)-(2×4)

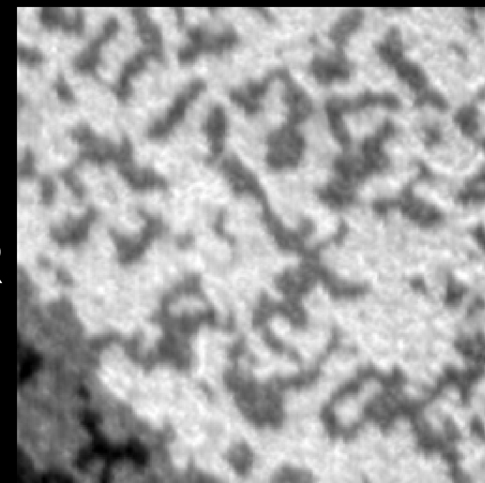


2 s Sb_2 at 400 °C



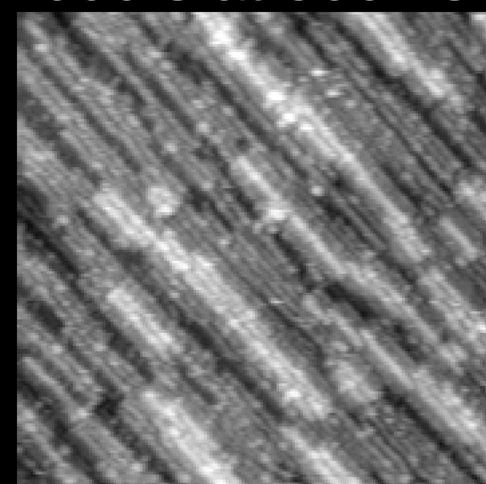
OR

30 s Sb_2



OR

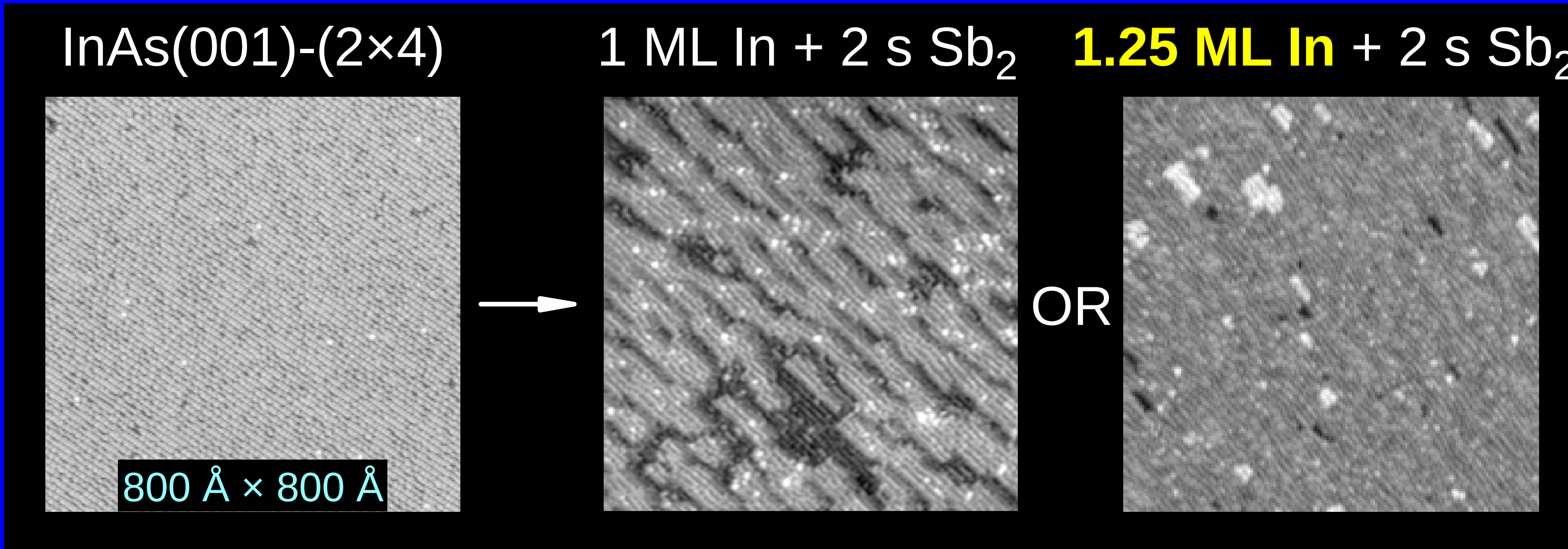
600 s at 500 °C

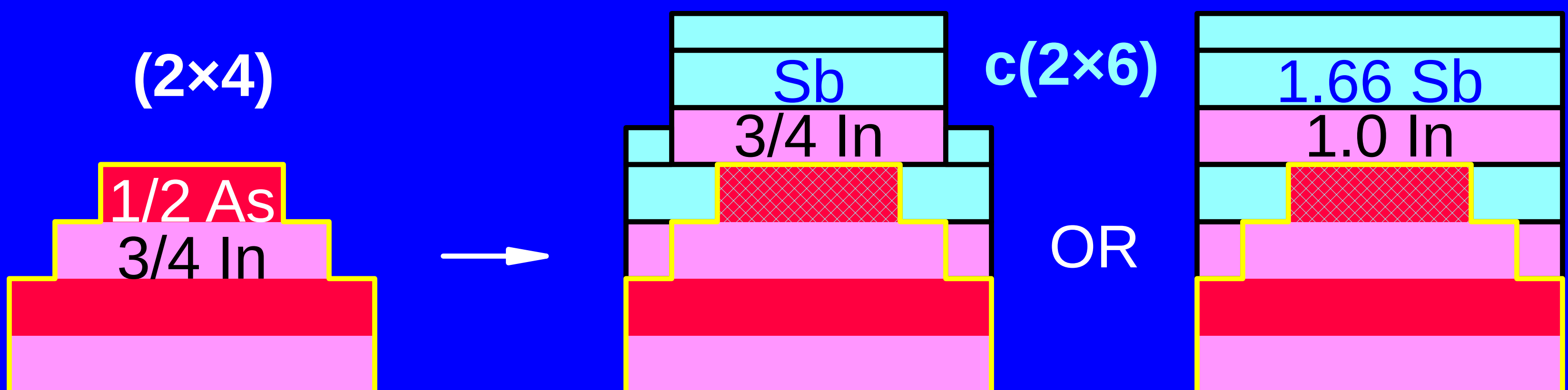


*Can **NOT** anneal out vacancies:*
get complex reconstruction.

Thermodynamics win!

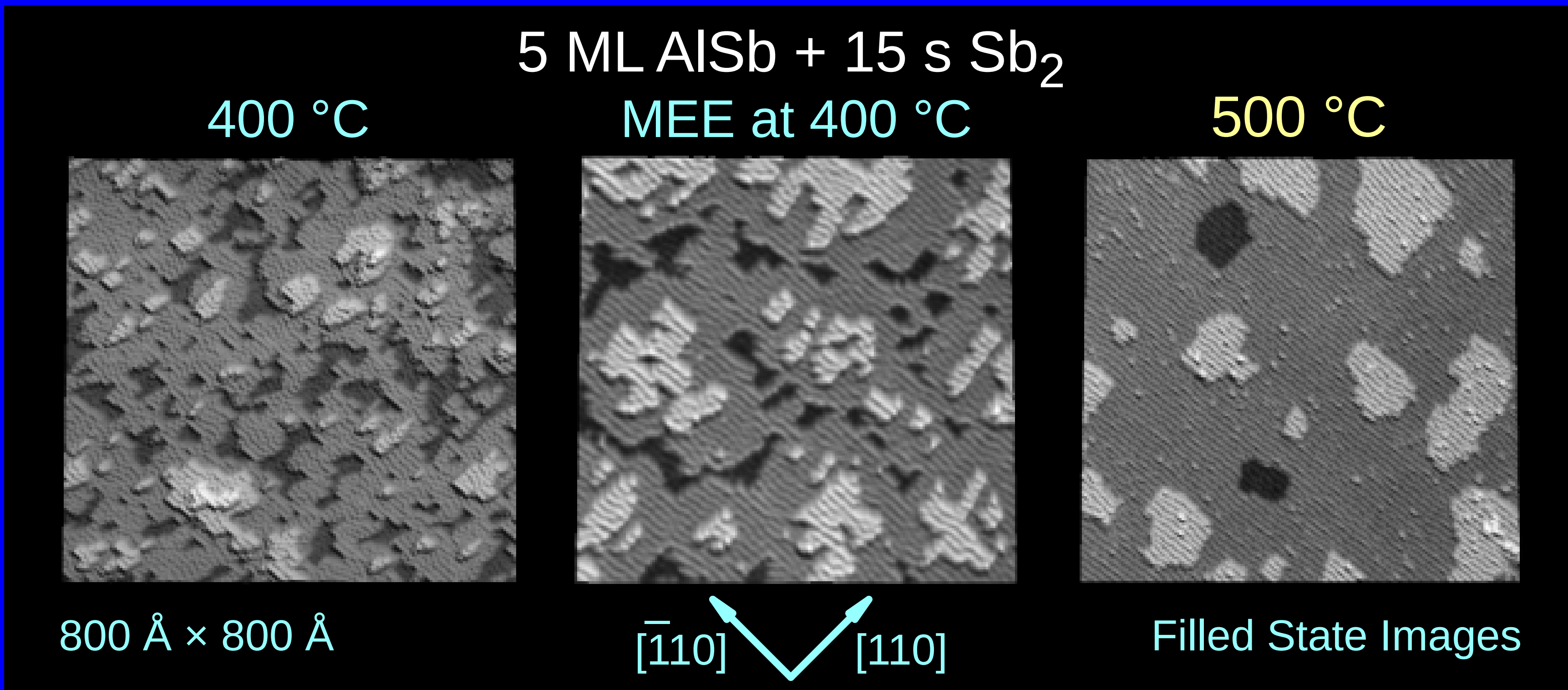
Origins of Interface Roughness: Sb/InAs

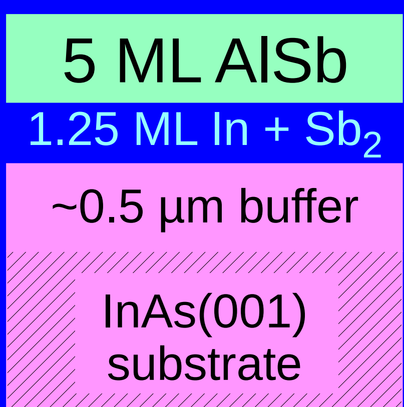




Roughness due to reconstruction stoichiometry!

Origins of Interface Roughness: AlSb/InAs

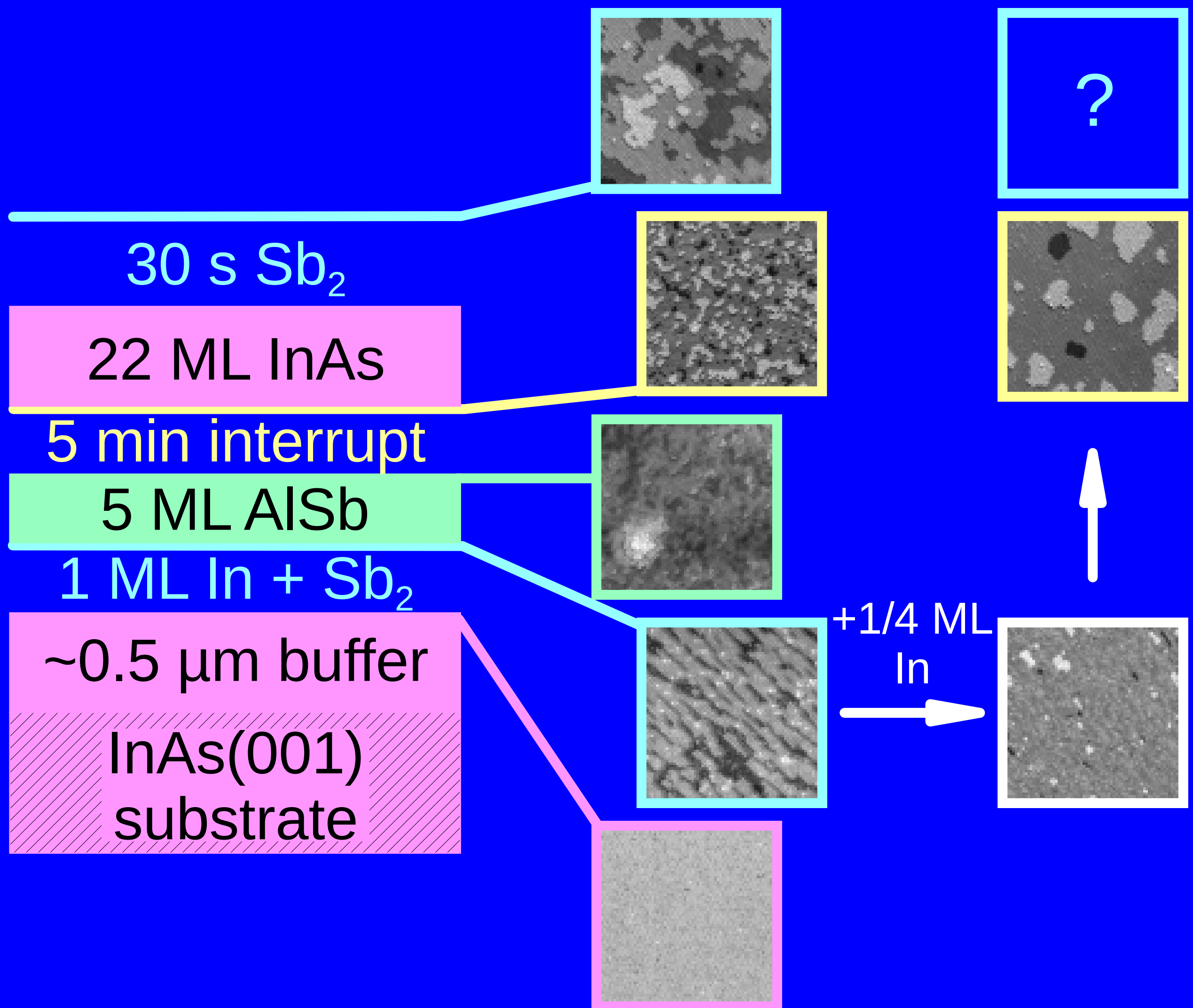




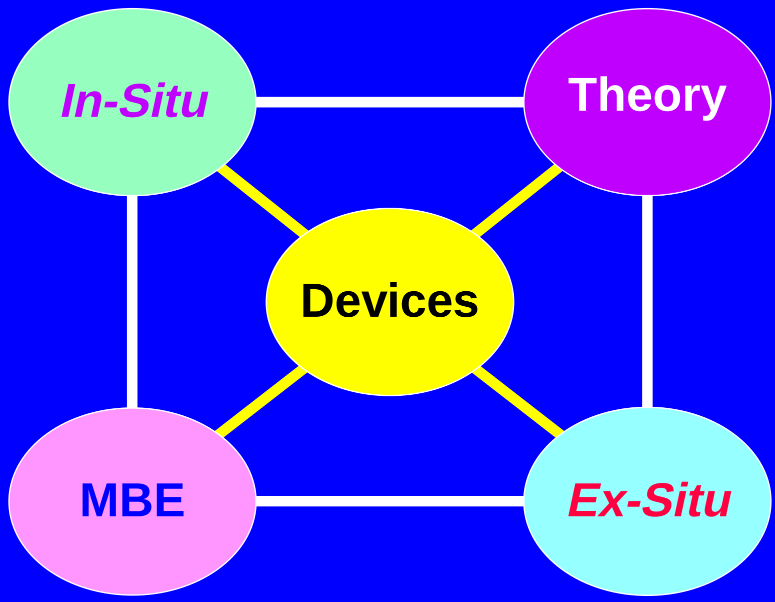
- Smoother starting surface + higher growth temp. improves 5 ML AlSb

Use higher T or MEE to smooth surface (higher T better).

Evolution of InAs/AlSb/InAs RTD Interfaces



Atomic-scale characterization = atomic-scale control!



MBE Under the Microscope

- Atomic-scale structure ***does*** matter
  - Can use MEE to compensate for III/V
- Complex interplay between kinetics and thermo.
  - "Obvious" approach does not always improve interface
- Need to better integrate theory, device character.

Work to be done – demonstrate improved devices!